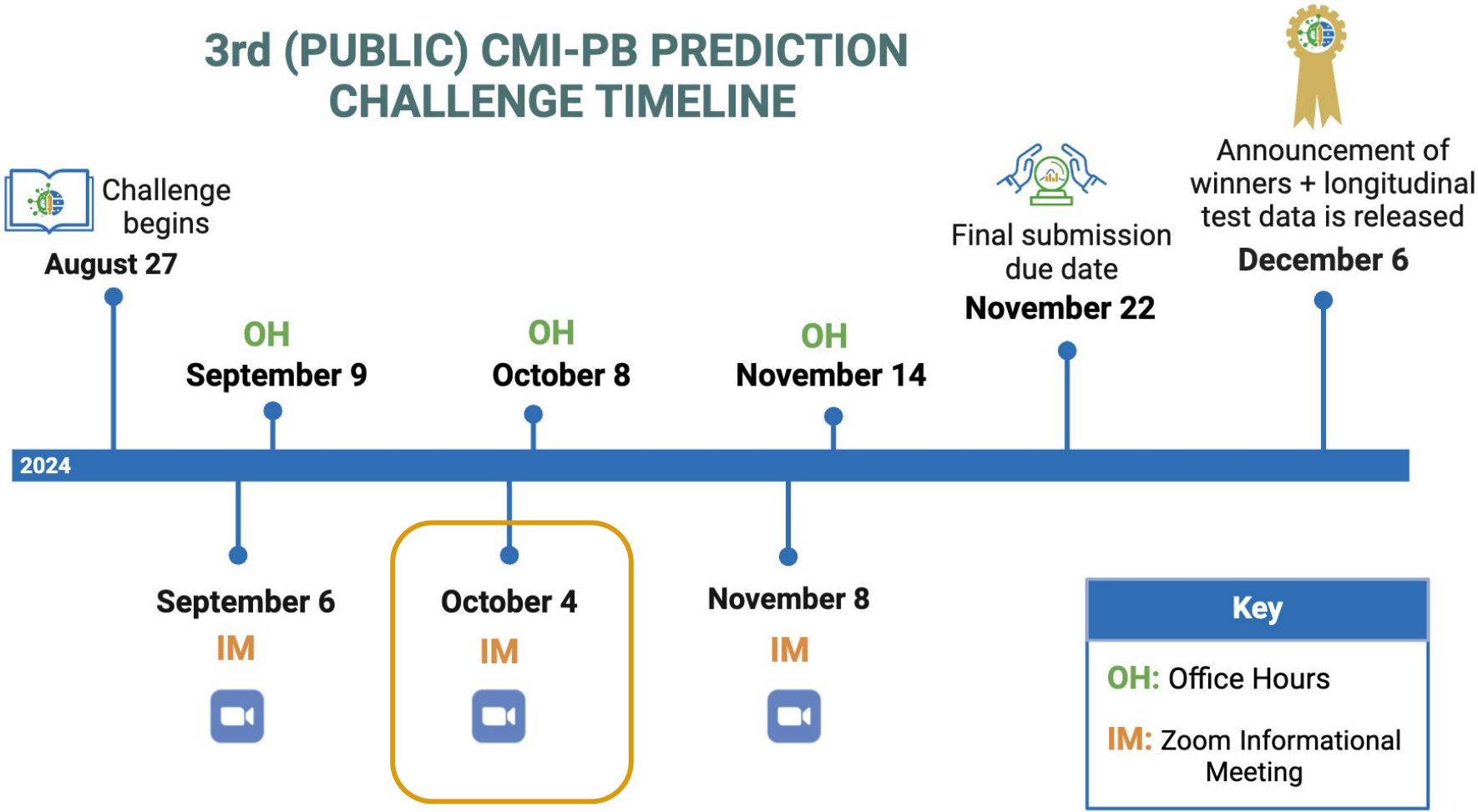
CMI-PB Prediction Challenge

2nd Informational Session
Oct 4th, 2024

La Jolla Institute for Immunology

CMI-PB
COMPUTATIONAL MODELS OF IMMUNITY
PERTUSSIS BOOST

3rd (PUBLIC) CMI-PB PREDICTION CHALLENGE TIMELINE



Agenda for Today's Session

1. Bonus Task
2. Other Updates
3. Submission Process
4. Reminders
5. Q & A

Agenda for Today's Session

1. **Bonus Task**
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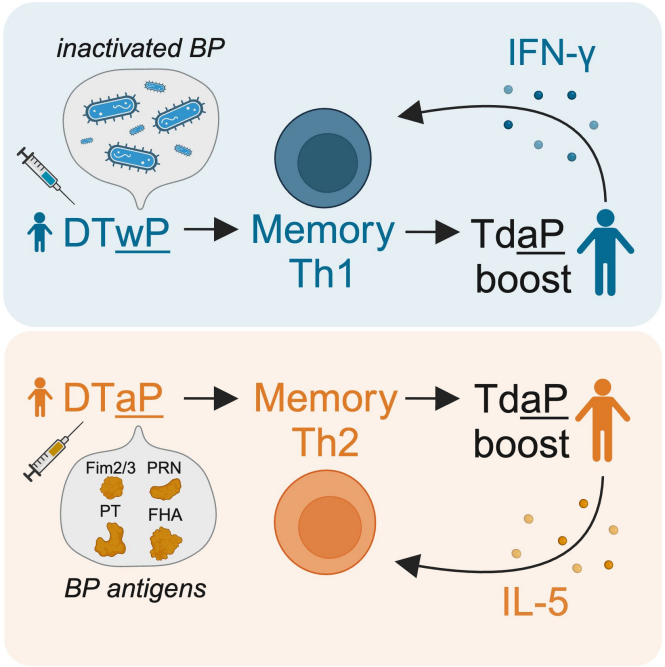
Bonus task: Background

A T-cell response task



- wP vaccination is associated with more durable protective immunity and a Th1-polarized memory T cell response compared to aP vaccination.
- Multi-omics analysis identified transcriptional changes and elevated IFN-γ levels post-booster as key correlates of Th1-polarized T cell responses, particularly in wP-primed individuals.
- The early interferon response observed in wP-primed individuals suggests that stimulating the interferon pathway during vaccination could enhance Th1 memory T cell responses in aP-primed individuals.

bioRχiv
THE PREPRINT SERVER FOR BIOLOGY

Th1 polarization in *Bordetella pertussis* vaccine responses is maintained through a positive feedback loop

Lisa Willemsen, Jiyeun Lee, Pramod Shinde, Ferran Soldevila, Minori Aoki, Shelby Orfield, Mari Kojima, Ricardo da Silva Antunes, Alessandro Sette, Bjoern Peters

doi: https://doi.org/10.1101/2024.08.05.606623

Bonus task: Task and Prize

A T-cell response task

- The bonus prediction task is separate from the main challenge and will be evaluated independently.
- Participation in the bonus task is optional.
- Submission deadline: Nov 22, 2024
- Task: Predict and rank individuals based on their Th1/Th2 (IFN-γ/IL-5) polarization ratio on day 30 post-booster vaccination (Task 4.1).
- Prize: A $500 cash prize will be awarded to the task winner.
- Submissions with a significant correlation coefficient may earn co-authorship in the resulting manuscript.
- Revised submission file: here

Revised Tasks list

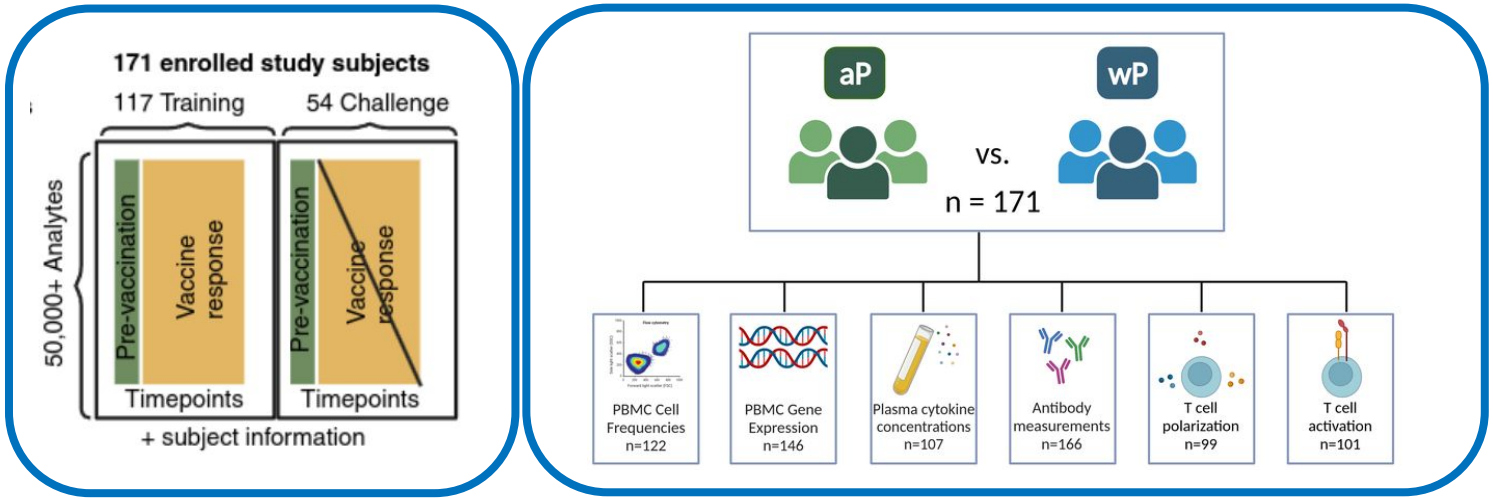
1) Antibody level tasks
1.1) Rank the individuals by IgG antibody levels against pertussis toxin (PT) that we detect in plasma 14 days post booster vaccinations.
1.2) Rank the individuals by fold change of IgG antibody levels against pertussis toxin (PT) that we detect in plasma 14 days post booster vaccinations compared to titer values at day 0.

2) Cell frequency tasks
2.1) Rank the individuals by predicted frequency of Monocytes on day 1 post boost after vaccination.
2.2) Rank the individuals by fold change of predicted frequency of Monocytes on day 1 post booster vaccination compared to cell frequency values at day 0.

3) Gene expression tasks
3.1) Rank the individuals by predicted gene expression of *CCL3* on day 3 post-booster vaccination.
3.2) Rank the individuals by fold change of predicted gene expression of *CCL3* on day 3 post booster vaccination compared to gene expression values at day 0.

4) T-cell response task (A Bonus task)
4.1) Rank the individuals by predicted Th1/Th2 (IFN-γ/IL-5) polarization ratio on day 30 post-booster vaccination.

Overview of the CMI-PB Challenge data



The data is split into two groups:

- **Training dataset (2020, 2021, 2022)**: Used to build models, including known outcomes ("ground truth"). Features are based on multi-omics readouts and demographic data, with potential for feature engineering.
- **Challenge dataset (2023)**: Used to evaluate model performance on unseen data. The task is to predict vaccine response outcomes without provided ground truth.

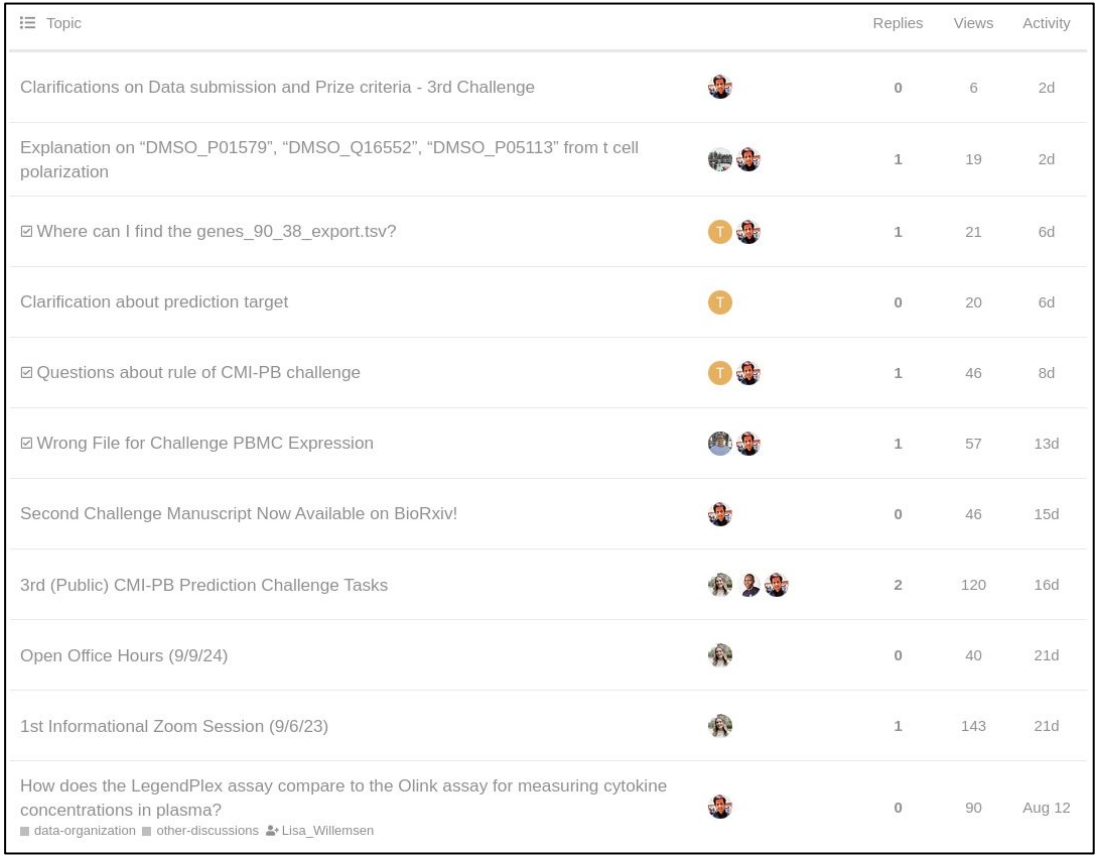
Challenge related information and Data access is provided via the CMI-PB website

CMI-PB Challenge Data: Raw and Processed Data

- The dataset comprises three multi-omics datasets (from 2020, 2021, and 2022) and the challenge dataset (2023).
- The data require careful processing and normalization to generate computable matrices suitable for model development.
- While data processing and normalization approaches can vary depending on user preferences, the CMI-PB team has provided a standardized data processing method inspired by the approach used in the 2nd CMI-PB challenge.
- Pipeline: RPub and GitHub

Data Access: https://www.cmi-pb.org/downloads/cmipb_challenge_datasets/current/3rd_challenge/

Recap of posts on Solutions Center



Topic	Replies	Views	Activity
Clarifications on Data submission and Prize criteria - 3rd Challenge	0	6	2d
Explanation on “DMSO_P01579”, “DMSO_Q16552”, “DMSO_P05113” from t cell polarization	1	19	2d
☑ Where can I find the genes_90_38_export.tsv?	1	21	6d
Clarification about prediction target	0	20	6d
☑ Questions about rule of CMI-PB challenge	1	46	8d
☑ Wrong File for Challenge PBMC Expression	1	57	13d
Second Challenge Manuscript Now Available on BioRxiv!	0	46	15d
3rd (Public) CMI-PB Prediction Challenge Tasks	2	120	16d
Open Office Hours (9/9/24)	0	40	21d
1st Informational Zoom Session (9/6/23)	1	143	21d
How does the LegendPlex assay compare to the Olink assay for measuring cytokine concentrations in plasma? ■ data-organization ■ other-discussions Lisa_Willemsen	0	90	Aug 12

Clarifications on Data Submission and Prize criteria

Clarifications on Data submission and Prize criteria - 3rd Challenge

3rd (Public) Challenge

Pramod 2d

Reuse of existing models:

- Contestants can use models/code from the first and second challenges as inspiration or apply similar techniques. Developing a new model that builds on past methods or using these experiences to make informed decisions is encouraged. While there are no strict rules on reusing these models, we encourage innovation rather than exact replication.
- After the conclusion of the 3rd Challenge on November 22, 2024 you are free to publish your developed model and findings. We encourage participants to share their models and insights with the broader scientific community.

Using external data:

- Contestants may use external datasets or predictors when building and evaluating their models. However, since it is important to disclose these details in our analyses and our manuscripts, we kindly request that they describe their approach to incorporating external data and predictors to ensure clarity for others when the team reaches out for your model information.

Multiple submissions/models:

- Contestants can submit as many submissions as they would like over the course of the challenge. The most recent submission by the deadline (November 22, 2024) will be counted as your final submission and will be evaluated accordingly by the CMI-PB Team.
- It is possible to combine predictions from different models into one submission.
- If contestants would like to submit multiple final submissions, we ask that contestants create a separate CMI-PB account for each submission. But we ask that no submitter is involved in more than 3 submissions.

Receiving your Prize:

- You must submit your code to the CMI-PB GitHub within 1 week of the winners announcement to receive the cash prize (top 3 winners).
- Toward the end of the challenge, we will collect information regarding your models to help analyze and develop our manuscript. Contestants will receive an Excel template designed to guide them through questions related to their modeling approach. While all winners are required to submit these summaries, we strongly encourage all contestants to provide their model summaries. Your contributions are invaluable in showcasing the diverse methodologies and innovations that have emerged throughout this challenge.

Feel free to let us know if contestants need clarification on any other topics regarding 3rd challenge.

Agenda for Today's Session

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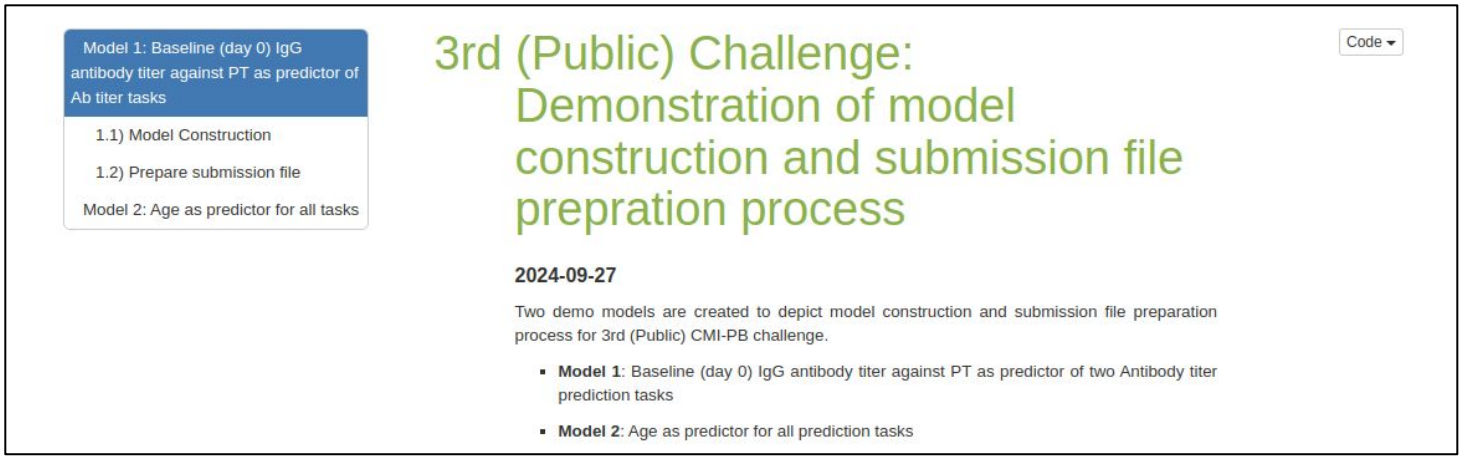
3. **Submission Process**
4. Reminders
5. Q & A

Submission Process Demonstration

https://www.cmi-pb.org/

Submission Process Demonstration

- We established two simple demo models that set a baseline of what more complex models should outperform.
- Model 1: Captures that pre-vaccination levels of antibody titer readouts are highly correlated with post-vaccination levels of the same readouts
- Model 2: Predicting vaccine responses solely based on the chronological age of the subject (the older, the worse) outperformed a lot of other models in predicting the antibody response to the Tdap vaccination



https://rpubs.com/pshinde/Public-CMI-PB-Challenge-Demo-Model-Construction-Submission-Process

3rd (Public) CMI-PB Challenge

Revolutionizing computational modelling approach for immune response prediction

Submission Deadline: 22nd Nov, 2024

Sign up to receive more information - here

Learn more: Prediction tasks, Training data, Challenge data, 1st Challenge, 2nd Challenge

The mission of CMI-PB is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of Pertussis booster vaccination.

LEARN ABOUT CMI-PB

- The NIH funded CMI network
- A community prediction challenge
- Pertussis (Whooping Cough)
- Pertussis vaccination
- Annual prediction challenges

UNDERSTAND THE DATA

- Study outline
- Sample and data collection
- Data standardization
- Database schema
- Terminology

ACCESS THE DATA

- Data composition
- Use the API in your programs
- Download data (SFTP)

PREDICTION CHALLENGE

- Data and resources
- Prediction challenge tasks
- Examples of models
- Submission instructions
- Submit prediction

TEACHING MATERIALS

- Overview
- Educational Resources
- Contact

SOLUTIONS CENTER

- Access tasks for 3rd challenge
- Data preprocessing questions
- FAQ: 3rd challenge

3rd (Public) CMI-PB Challenge Submission

Table of contents

Welcome to the 3rd (Public) CMI-PB challenge! Please follow the steps below to submit your prediction challenge. If you have any issues, go to our solutions center to post any questions and we will get back to you.

Step 1: Prepare your submission file

1. Create a model and run your analysis.
2. Download the submission template. Note that we only accept submissions in the given Tab-separated values (TSV) file format.
3. Enter your prediction in the prescribed format.

Step 2: Submit your file

1. Take your filled out submission template, and make sure it is saved in tsv format on your computer.
    a. Your submission should be a TSV file with 54 rows including a header and 10 columns. The maximum allowed file size is 100 KB.
    b. Example submission files are available here.
2. Click on the "Choose File" button below and select the tsv template you have filled out.
3. Click the "Submit" button.

Select a submission file: Choose File No file chosen

I'm not a robot reCAPTCHA Privacy - Terms

Submit

Submission File Errors

SubjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank	1.2) IgG-PT-D14-FC-Rank	2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
119	23	Female	aP		39			ABC	8	37
120	27	Female	wP		45			39	31	5
121	22	Female	aP		3			5	33	22
122	23	Female	aP		18			34	23	12
123	26	Female	wP		47			8	30	43
124	22	Male	aP		42			16	43	8
125	29	Male	wP		17			41	25	26
126	29	Male	wP		2			27	38	4
127	26	Female	aP		1			48	50	19
128	28	Female	wP		9			2	42	15
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131	24	Female	aP		8			26	51	34
132	27	Male	wP							
133	25	Female	aP							
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135	27	Male	wP							
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137	24	Female	aP							
138	22	Male	aP							
139	29	Female	wP							
140	21	Female	aP							
141	26	Female	wP							

Submission file error: contains non-numeric values

Select a submission file: Choose File No file chosen

Column 3.1) CCL3-D3-Rank contains non-numeric values that were converted to NaN. ✕

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Submit

SubjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank	1.2) IgG-PT-D14-FC-Rank	2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
119	23	Female	aP							
120	27	Female	wP							
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122	23	Female	aP							
123	26	Female	wP							
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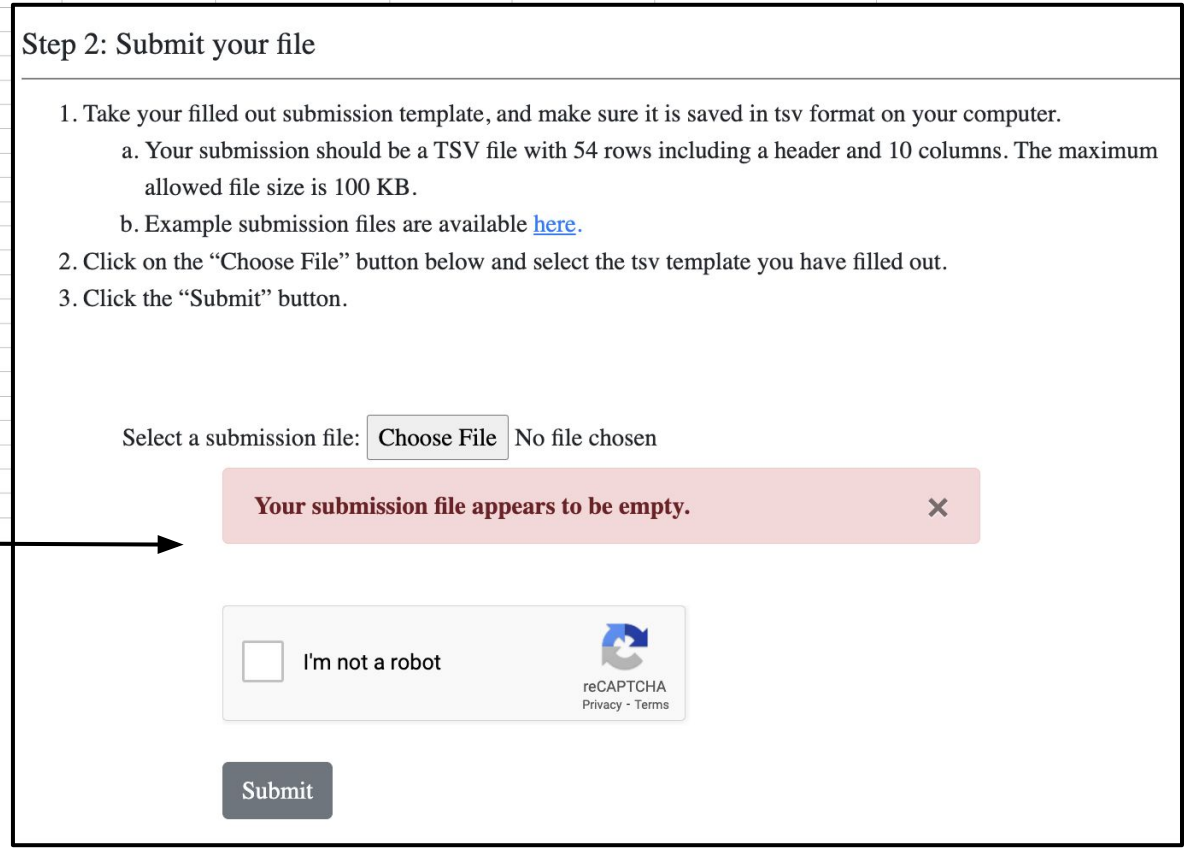
143	19	Female	aP							

Submission file error: empty file



bjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank		2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
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137	24	Female	aP	11						
138	22	Male	aP	48						
139	29	Female	wP	12						
140	21	Female	aP	13						
141	26	Female	wP	29						
142	31	Female	aP	44						
143	19	Female	aP	50						
144	23	Female	aP	30						
145	20	Male	aP	33						

Submission file error: missing/incorrect header

Step 2: Submit your file

1. Take your filled out submission template, and make sure it is saved in tsv format on your computer.
   a. Your submission should be a TSV file with 54 rows including a header and 10 columns. The maximum allowed file size is 100 KB.
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Select a submission file: Choose File No file chosen

The header does not align with the expected columns specified in the submission template ×

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Submit

SubjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank	1.2) IgG-PT-D14-FC-Rank	2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
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136	27	Female	wP	49		5				
137	24	Female	aP	37		13				
138	22	Male	aP	47		37				
139	29	Female	wP	33		33				
140	21			35		38				
141	26			44		29				
142	31			54		18				
143	19			5		17				
144	23			52		45				
145	20	Male	aP	17		50				

Submission file with multiple errors

Select a submission file: Choose File No file chosen

Column 1.1) IgG-PT-D14-titer-Rank contains non-numeric values that were converted to NaN. ×

Column 1.1) IgG-PT-D14-titer-Rank: All rank values must be within the range (1-54) or NaN. ×

Column 1.2) IgG-PT-D14-FC-Rank contains non-numeric values that were converted to NaN. ×

Column 1.2) IgG-PT-D14-FC-Rank: All rank values must be within the range (1-54) or NaN. ×

Column 2.1) Monocytes-D1-Rank: All rank values must be within the range (1-54) or NaN. ×

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Submit

Successful Submissions

Submission with all tasks

SubjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank	1.2) IgG-PT-D14-FC-Rank	2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
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120	27	Female	wP	27	45	27	45	39	31	5
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122	23	Female	aP	12	18	12	19	34	23	12
123	26	Female	wP	39	47	25	11	8	30	43
124	22	Male	aP	7	42	35	34	16	43	8
125	29	Male	wP	34	17	42	24	41	25	26
126	29	Male	wP	15	2	10	40	27	38	4
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140	21	Female	aP	35	13	38	52	45	45	10
141	26	Female	wP	44	29	29	18	30	34	27
142	31	Female	aP	54	44	18	50	20	12	25
143	19	Female	aP	5	50	17	12	14	9	52
144	23	Female	aP	52	30	45	46	36	1	3
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146	31	Male	wP	46	4	14	39	4	41	50
147	23	Female	aP	43	7	21	35	31	15	40
148	35	Male	wP	19	24	36	3	15	39	38
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150	32	Male	wP	51	38	44	20	7	53	49
151	31	Female	wP	2	5	46	22	13	21	18

*Populated with random numbers

Submission with all tasks completed except bonus task

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PERTUSSIS BOOST

SubjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank	1.2) IgG-PT-D14-FC-Rank	2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
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121	22	Female	aP	26	3	19	7	5	33	
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123	26	Female	wP	39	47	25	11	8	30	
124	22	Male	aP	7	42	35	34	16	43	
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132	27	Male	wP	24	40	11	2	50	28	
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138	22	Male	aP	47	48	37	30	12	7	
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149	32	Female	wP	8	16	4	1	28	22	
150	32	Male	wP	51	38	44	20	7	53	
151	31	Female	wP	2	5	46	22	13	21	

*Populated with random numbers

Submission with two tasks

CMI-PB
COMPUTATIONAL MODELS OF IMMUNITY
PERTUSSIS BOOST

SubjectID	Age	BiologicalSexAtBirth	VaccinePrimingStatus	1.1) IgG-PT-D14-titer-Rank	1.2) IgG-PT-D14-FC-Rank	2.1) Monocytes-D1-Rank	2.2) Monocytes-D1-FC-Rank	3.1) CCL3-D3-Rank	3.2) CCL3-D3-FC-Rank	4.1) IFNG/IL5-Polarization-D30-Rank
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120	27	Female	wP		45				31	
121	22	Female	aP		3				33	
122	23	Female	aP		18				23	
123	26	Female	wP		47				30	
124	22	Male	aP		42				43	
125	29	Male	wP		17				25	
126	29	Male	wP		2				38	
127	26	Female	aP		1				50	
128	28	Female	wP		9				42	
129	31	Male	wP		10				4	
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131	24	Female	aP		8				51	
132	27	Male	wP		40				28	
133	25	Female	aP		32				49	
134	32	Male	wP		37				29	
135	27	Male	wP		25				20	
136	27	Female	wP		14				16	
137	24	Female	aP		11				13	
138	22	Male	aP		48				7	
139	29	Female	wP		12				27	
140	21	Female	aP		13				45	
141	26	Female	wP		29				34	
142	31	Female	aP		44				12	
143	19	Female	aP		50				9	
144	23	Female	aP		30				1	
145	20	Male	aP		33				54	
146	31	Male	wP		4				41	
147	23	Female	aP		7				15	
148	35	Male	wP		24				39	
149	32	Female	wP		16				22	
150	32	Male	wP		38				53	
151	31	Female	wP		5				21	

*Populated with random numbers

3rd (Public) CMI-PB challenge Submission

Your submission has been recorded successfully. A confirmation email has been sent to you. Thank you!

Useful links:

- CMI-PB home

Please let us know if you have any questions at our CMI-PB solutions center.

Supported by a grant from the National Institutes of Health (NIH U01 AI150753) |

Regarding your 3rd (Public) CMI-PB challenge submission External Inbox ×

submission@cmi-pb.org via lji.org
to me, aazhan

9:44 AM (6 hours ago)

CMI-PB
COMPUTATIONAL MODELS OF IMMUNITY
PERTUSSIS BOOST

Welcome to the 3rd CMI-PB Prediction Challenge

Dear sorfield@lji.org,

Thank you for entering your submission to the 3rd CMI-PB Prediction challenge. Your submission is now successfully recorded.

The submitted file is attached here for your reference. Feel free to access all your past submissions here. If you ever change your mind and want to re-submit, please make sure to enter all your answers in the sheet again as your new submission overrides all previous submissions.

We look forward to reviewing your results! In the meantime, please let us know if you have any questions at our CMI-PB solutions center.

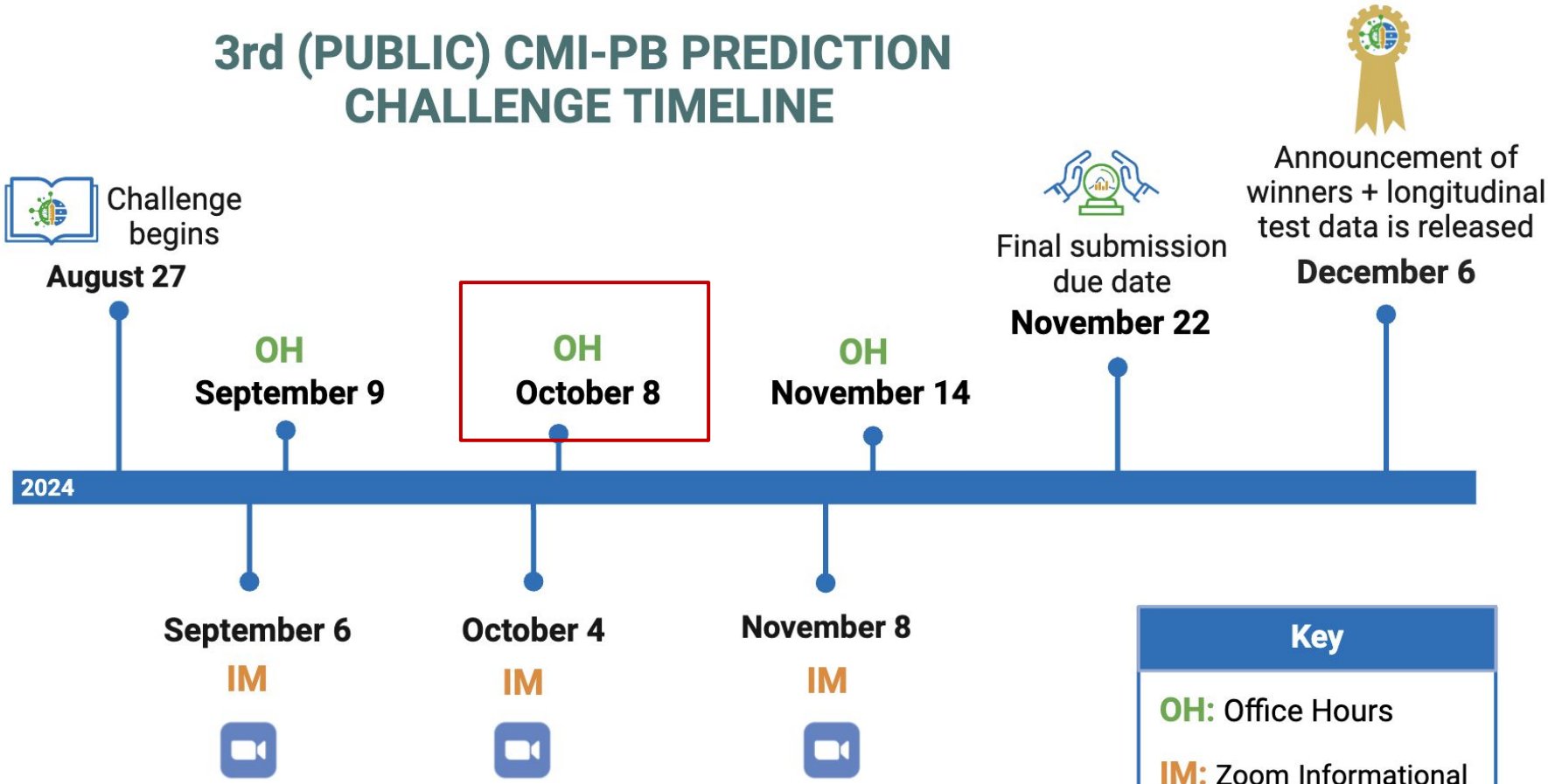
Best wishes,
CMI-PB Team

You will receive an email confirmation once your submission is received.

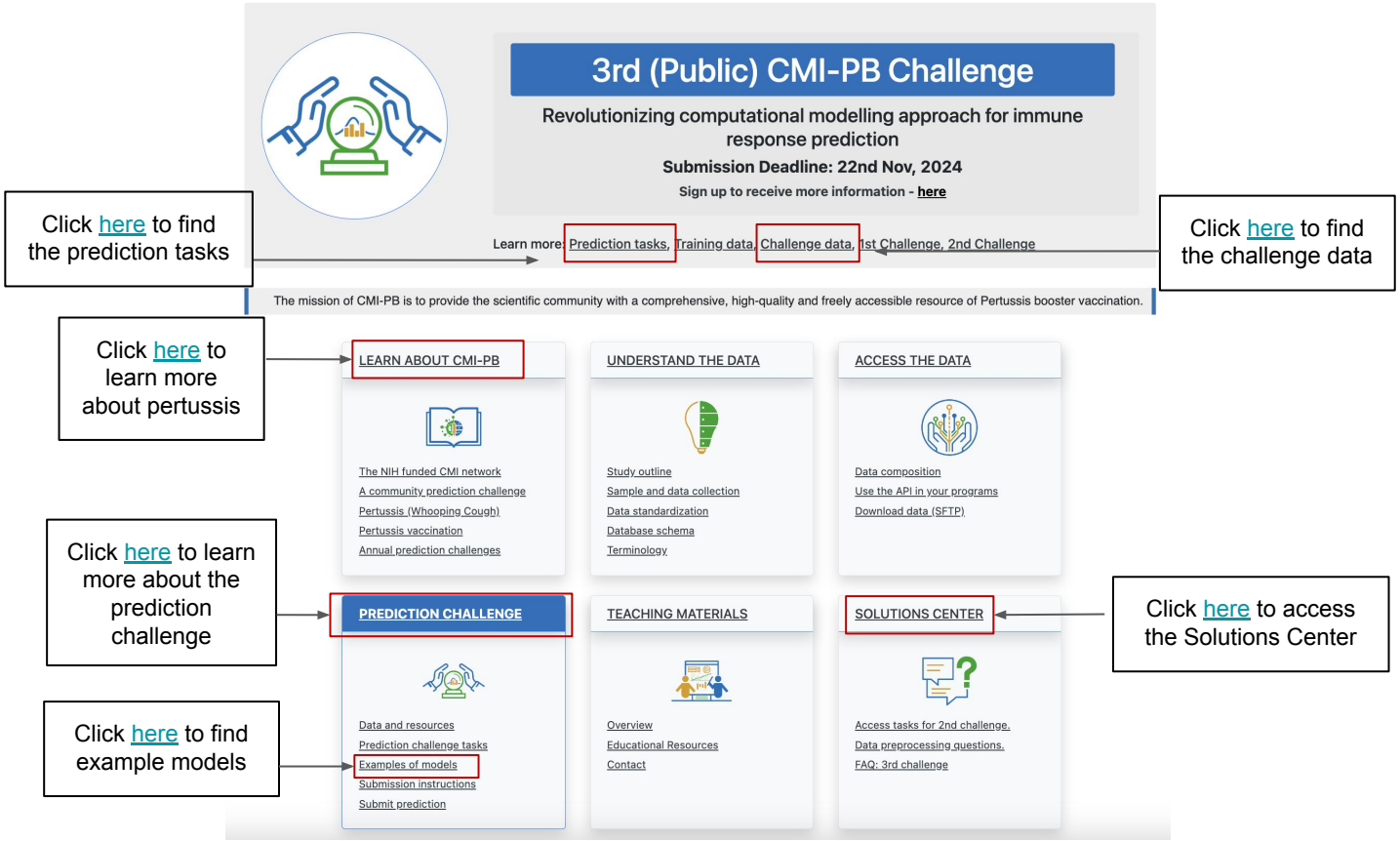
Agenda for Today's Session

1. Bonus Task
2. Other Updates
3. Submission Process
4. **Reminders**
5. Q & A

3rd (PUBLIC) CMI-PB PREDICTION CHALLENGE TIMELINE



Summary of other resources on the site



The CMI-PB team

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Kleinstein Lab (Yale)

- Expertise: A combination of "big data" analysis and immunology domain.
- Collaborating on data and models being released to the community to support reproducibility and the prediction contest, and also participate in the prediction challenge.

Steven Kleinstein
Jeremy Gygi
Leying Guan
Anna Konstorum

Grant Lab (UCSD)

- Expertise: the use of computational approaches, based on both biophysics and bioinformatics, to study the structure, function and evolution of key biological macromolecules.
- Dr. Grant will engage and advise over 40 biology graduate students in the CMI-PB Prediction Challenge.

Barry Grant

Ay Lab (LJI)

- Expertise: Development of bioinformatics tools that utilize high-dimensional and high-throughput datasets to deduce insights into chromatin conformation, genetic variation, and the regulation of gene expression.
- The Ay lab is focused on developing predictive machine learning models, which will serve as examples and baselines for participants in the CMI-PB challenge.

Ferhat Ay
Joaquin Reyna

Peters Lab (LJI)

- Expertise: Both experimental and computational studies to better understand human immune responses in the context of infectious diseases, allergy, cancer and vaccines.
- The team is responsible for the generation of experimental data, making it accessible in a central and standardized fashion, and coordinating the creation and coordination of the prediction contest.

Bjoern Peters
Jason Greenbaum
James Overton
Brendan Ha
Pramod Shinde
Mari Kojima
Rasteh Haji Kazem Nili
Jiyeun Lee
Lisa Willemsen
Shelby Orfield

And thank you to the Sette Lab, Crotty lab, LJI Clinical Core, LJI Bioinformatics Core

Past & Current CMI-PB team members

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PERTUSSIS BOOST


Bjoern Peters


Steven Kleinstein


Ferhat Ay


Barry Grant


Shane Crotty


Alessandro Sette


Pramod Shinde


Shelby Orfield


Lisa Willemsen


Leying Guan


Joaquin Reyna


Mari Kojima


Ferran Soldevila


Aaron Ren


Jason Greenbaum


Brendan Ha


Jiyeun Lee


Ricardo De Silva Antunes


Jeremy Gygi


Rasteh Nili


Minori Aoki


Jian Xing


Anna Konstorum

Agenda for Today's Session

1. Bonus Task
2. Other Updates
3. Submission Process
4. Reminders
5. Q & A

Questions?

Please post your questions on https://discuss.cmi-pb.org/
under the 3rd Public Challenge

We will be hosting an open office hour session via Zoom on **Tuesday, October 8th 9:00am-10:00am PT/ 12:00pm-1:00pm ET**.

Feel free to drop by if you have any questions!
Zoom information is available on the Solutions Center here.